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Optimal Runge-Kutta Schemes for High-order Spatial and Temporal Discretizations

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Outline

- **Introduction**
- **Governing Equations**
 - Spatial Discretizations
 - Temporal Discretizations
- **Von Neumann Analysis (VNA)**
- **Computational Results**
 - One-dimensional Wave
 - Three-dimensional Vortex
- **Conclusions and Future Work**



Introduction

- High-order in space is now commonplace
- High-order in time... not so much...
- Is this sufficient? Is high-order in time needed?
- Limiting Fact: There are no A -stable backward-difference formula (BDF) methods with $> 2^{nd}$ -order accuracy
- Thus, multistage methods, like Runge-Kutta (RK) methods, must be used for 3^{rd} - and higher-order
- Explicit RK methods are not amenable to stiff problems

Objective: To find optimal diagonally-implicit Runge-Kutta time integrators for use with high-order spatial discretizations



Governing Equations



- **Dual Time Stepping:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H}$$

$$\mathbf{Q} = [\rho \quad \rho u_i \quad \rho e_0]^T$$

$$\mathbf{F}_i = [\rho u_i \quad \rho u_i u_j + p \delta_{ij} \quad u_i \rho h_0]^T \quad \text{where } h_0 = e_0 + \frac{p}{\rho}$$

- **Quasi-linear Form:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \underline{\mathbf{A}} \frac{\partial \mathbf{Q}}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H} \quad \underline{\mathbf{A}} = \frac{\partial \mathbf{F}_i}{\partial \mathbf{Q}} = \underline{\mathbf{M}} \underline{\Lambda} \underline{\mathbf{M}}^{-1}$$

$$\underline{\Lambda} = \text{diag} \{u_i + c, u_i, u_i - c\}$$

- **Residual Form:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \mathbf{R}_s(\mathbf{Q}) = 0 \quad \text{where} \quad \mathbf{R}_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}$$



Spatial Discretizations



- Central Differences with added artificial dissipation
- Central differences:

$$\left. \frac{\partial \Upsilon_j}{\partial x_i} \right|_{II} = \frac{\Upsilon_{j+1} - \Upsilon_{j-1}}{2\Delta x_i}$$

$$\left. \frac{\partial \Upsilon_j}{\partial x_i} \right|_{IV} = \frac{-\Upsilon_{j+2} + 8\Upsilon_{j+1} - 8\Upsilon_{j-1} + \Upsilon_{j-2}}{12\Delta x_i}$$

$$\left. \frac{\partial \Upsilon_j}{\partial x_i} \right|_{VI} = \frac{\Upsilon_{j+3} - 9\Upsilon_{j+2} + 45\Upsilon_{j+1} - 45\Upsilon_{j-1} + 9\Upsilon_{j-2} - \Upsilon_{j-3}}{60\Delta x_i}$$

where Υ could be \mathbf{F}_i or \mathbf{Q} depending on the form of the equations

- Scalar artificial dissipation:

$$\mathbf{R}_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \varepsilon_\eta \|\lambda\| \frac{\partial^\eta \mathbf{Q}}{\partial x_i^\eta} - \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}$$

where η is even and one more than the order of accuracy

$$\|\lambda\| = |u_i| + c \quad \varepsilon_{II} = \frac{\Delta x_i}{2}, \quad \varepsilon_{IV} = -\frac{\Delta x_i^3}{12}, \quad \varepsilon_{VI} = \frac{\Delta x_i^5}{60}.$$



Temporal Discretizations

- Runge-Kutta Methods:

c_1	a_{11}	a_{12}	a_{13}	\dots	$a_{1(s-1)}$	a_{1s}
c_2	a_{21}	a_{22}	a_{23}	\dots	$a_{2(s-1)}$	a_{2s}
c_3	a_{31}	a_{32}	a_{33}	\dots	$a_{3(s-1)}$	a_{3s}
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
c_{s-1}	$a_{(s-1)1}$	$a_{(s-1)2}$	$a_{(s-1)3}$	\dots	$a_{(s-1)(s-1)}$	$a_{(s-1)s}$
c_s	a_{s1}	a_{s2}	a_{s3}	\dots	$a_{s(s-1)}$	a_{ss}
<hr/>						
	b_1	b_2	b_3	\dots	b_{s-1}	b_s
	\hat{b}_1	\hat{b}_2	\hat{b}_3	\dots	\hat{b}_{s-1}	\hat{b}_s

$$t^k = t^n + c_k \Delta t \quad \mathbf{Q}^k = \mathbf{Q}^n - \Delta t \sum_{j=1}^s a_{kj} \mathbf{R}_s^j(\mathbf{Q}^j) \quad k = 1, 2, \dots, s$$

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n - \Delta t \sum_{j=1}^s b_j \mathbf{R}_s^j(\mathbf{Q}^j) \quad \hat{\mathbf{Q}}^{n+1} = \mathbf{Q}^n - \Delta t \sum_{j=1}^s \hat{b}_j \mathbf{R}_s^j(\mathbf{Q}^j)$$

$$\epsilon^{n+1} = \mathbf{Q}^{n+1} - \hat{\mathbf{Q}}^{n+1}$$



ESDIRK Methods

- Explicit first stage Singly-Diagonally
Implicit Runge-Kutta
 - Stiffly accurate
 - Second-order stage accuracy
 - FSAL – First is the Same As Last

$c_1 = 0$	0	0	...	0	0
c_2	a_{21}	λ	...	0	0
c_3	a_{31}	a_{32}	...	0	0
\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
c_{s-1}	$a_{(s-1)1}$	$a_{(s-1)2}$	$a_{(s-1)3}$	λ	0
$c_s = 1$	b_1	b_2	b_3	b_{s-1}	λ
	b_1	b_2	b_3	b_{s-1}	λ
	\hat{b}_1	\hat{b}_2	\hat{b}_3	\hat{b}_{s-1}	\hat{b}_s



ESDIRK3 and 4

0	0	0	0	0	0
$\frac{1767732205903}{2027836641118}$	$\frac{1767732205903}{4055673282236}$	$\frac{1767732205903}{4055673282236}$	$\frac{1767732205903}{4055673282236}$	$\frac{1767732205903}{4055673282236}$	$\frac{1767732205903}{4055673282236}$
$\frac{3}{5}$	$\frac{2746238789719}{10658868560708}$	$\frac{640167445237}{6845629431997}$	$\frac{1767732205903}{4055673282236}$	$\frac{1767732205903}{4055673282236}$	$\frac{1767732205903}{4055673282236}$
1	$\frac{1471266399579}{7840856788654}$	$\frac{4482444167858}{7529755066697}$	$\frac{11266239266428}{11593286722821}$	$\frac{11266239266428}{11593286722821}$	$\frac{1767732205903}{4055673282236}$
	$\frac{1471266399579}{7840856788654}$	$\frac{4482444167858}{7529755066697}$	$\frac{11266239266428}{11593286722821}$	$\frac{11266239266428}{11593286722821}$	$\frac{1767732205903}{4055673282236}$

Implicit, Third-order ESDIRK3

0	0	0	0	0	0	0
$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0
$\frac{83}{250}$	$\frac{8611}{62500}$	$\frac{1743}{31250}$	$\frac{1}{4}$	0	0	0
$\frac{31}{50}$	$\frac{5012029}{34652500}$	$\frac{654441}{2922500}$	$\frac{174375}{388108}$	$\frac{1}{4}$	0	0
$\frac{17}{20}$	$\frac{15267082809}{155376265600}$	$\frac{71443401}{120774400}$	$\frac{730878875}{902184768}$	$\frac{2285395}{8070912}$	$\frac{1}{4}$	0
1	$\frac{82889}{524892}$	0	$\frac{15625}{83664}$	$\frac{69875}{102672}$	$\frac{2260}{8211}$	$\frac{1}{4}$
	$\frac{82889}{524892}$	0	$\frac{15625}{83664}$	$\frac{69875}{102672}$	$\frac{2260}{8211}$	$\frac{1}{4}$

Implicit, Fourth-order ESDIRK4



Distribution A – Approved for public release; Distribution Unlimited



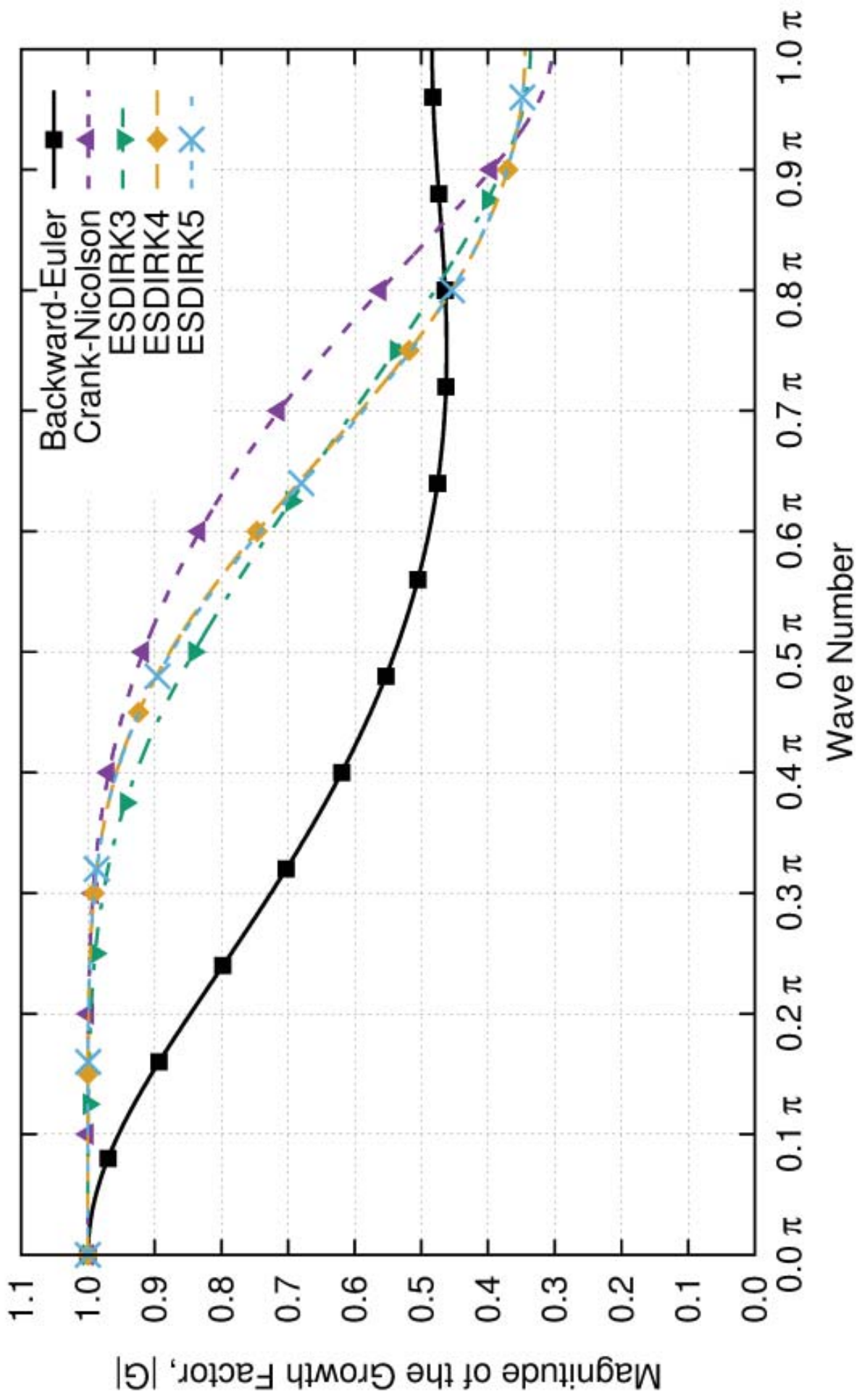
Von Neumann Analysis



- **Often used to study stability of schemes**
- **Von Neumann analysis is used to compare schemes for accuracy**
 - Dissipation error
 - Dispersion error
- **Assumes linear, periodic problems**
- **VNA theory and more results are in the associated paper**

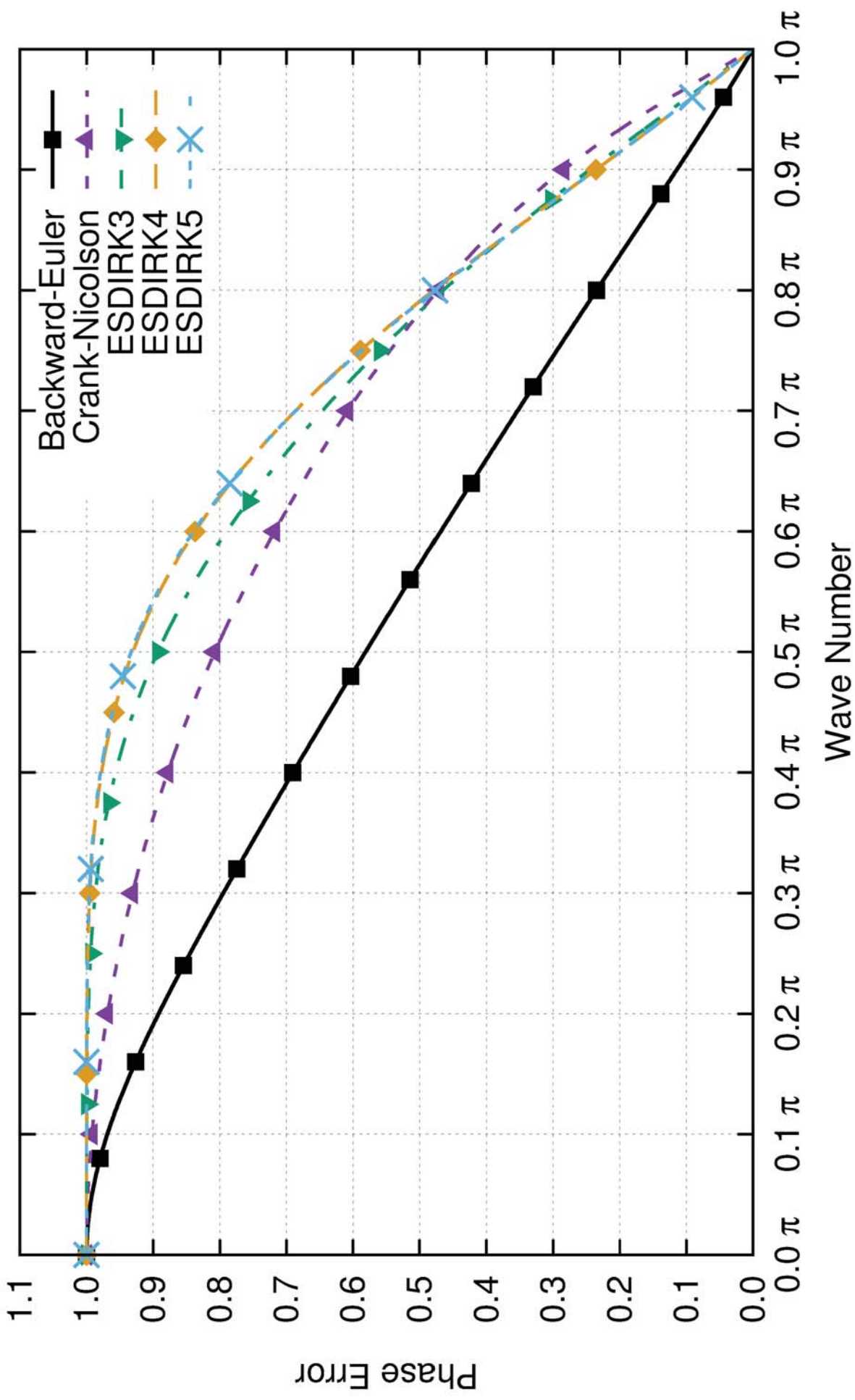


Dissipation, $CFL = 1.0$



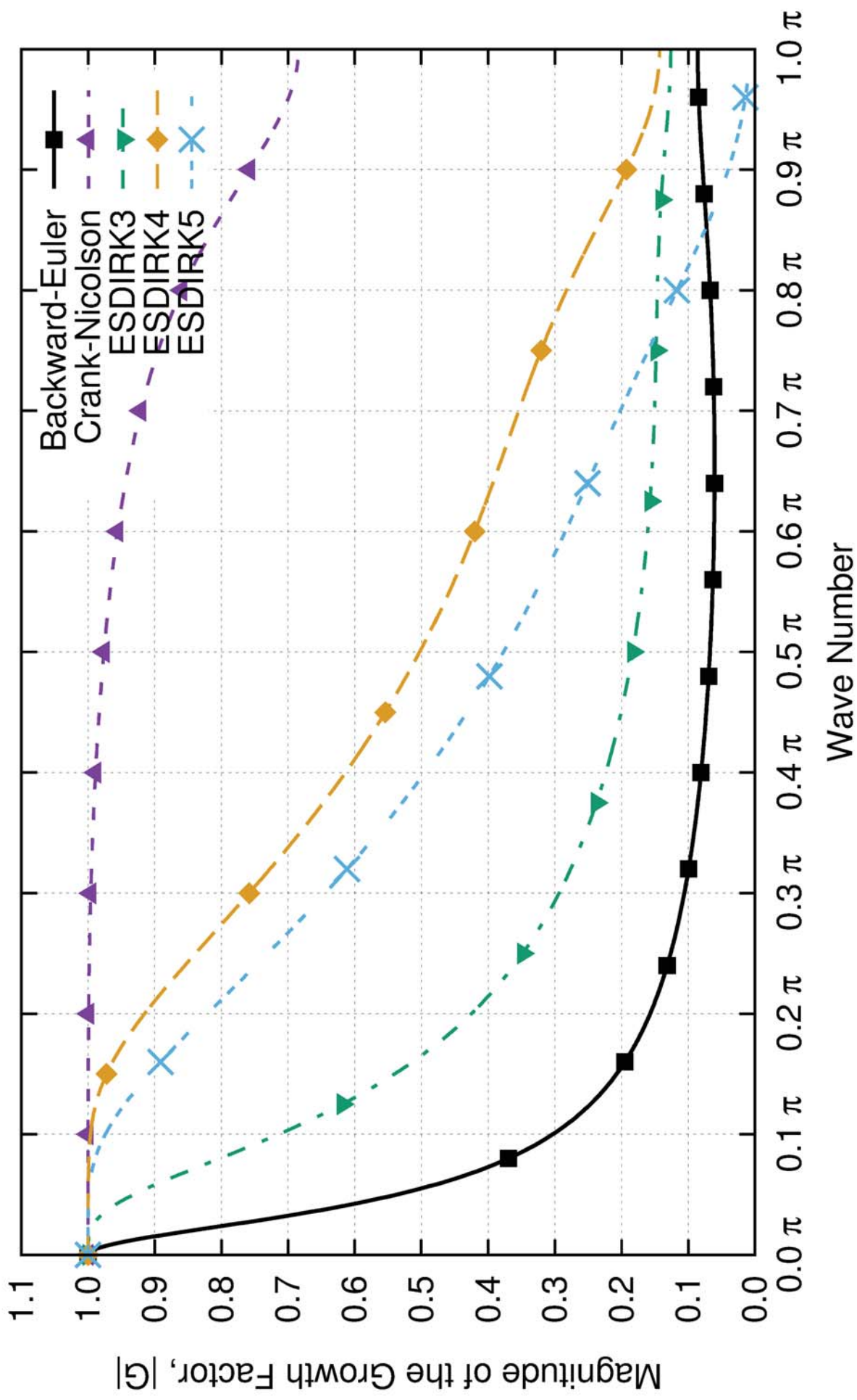


Dispersion, $CFL = 1.0$



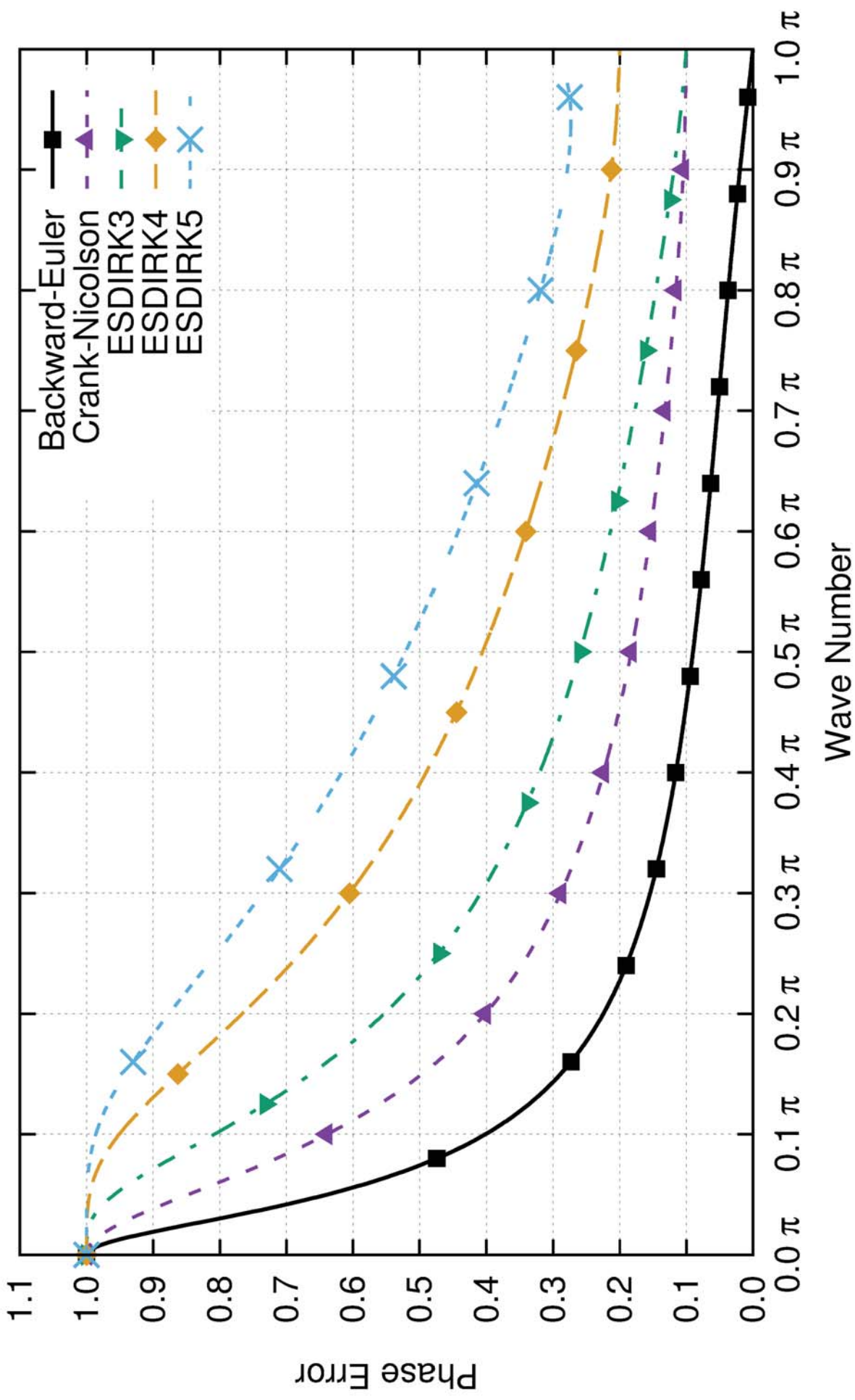


Dissipation, $CFL = 10.0$





Dispersion, $CFL = 10.0$





1-D Acoustic Wave



- **Unperturbed Mach number of 0.5**

$$\rho_{\infty} = 8.7077 \times 10^{-1} \frac{\text{kg}}{\text{m}^3}$$

$$\rho u_{\infty} = 1.7458 \times 10^2 \frac{\text{kg}}{\text{m}^2 \cdot \text{s}}$$

$$T_{\infty} = 400K$$

$$R_{\infty} = 2.871 \times 10^2 \frac{J}{\text{kg} \cdot K}$$

$$\gamma = 1.4$$

- **Perturbation wave - 20 points per wave resolution**

$$Q_o = Q_{\infty} + M \delta \hat{Q}_{u,u \pm c}$$

$$\delta \hat{Q}_{u,u \pm c} = \hat{\delta} \cdot \cos(kx)$$

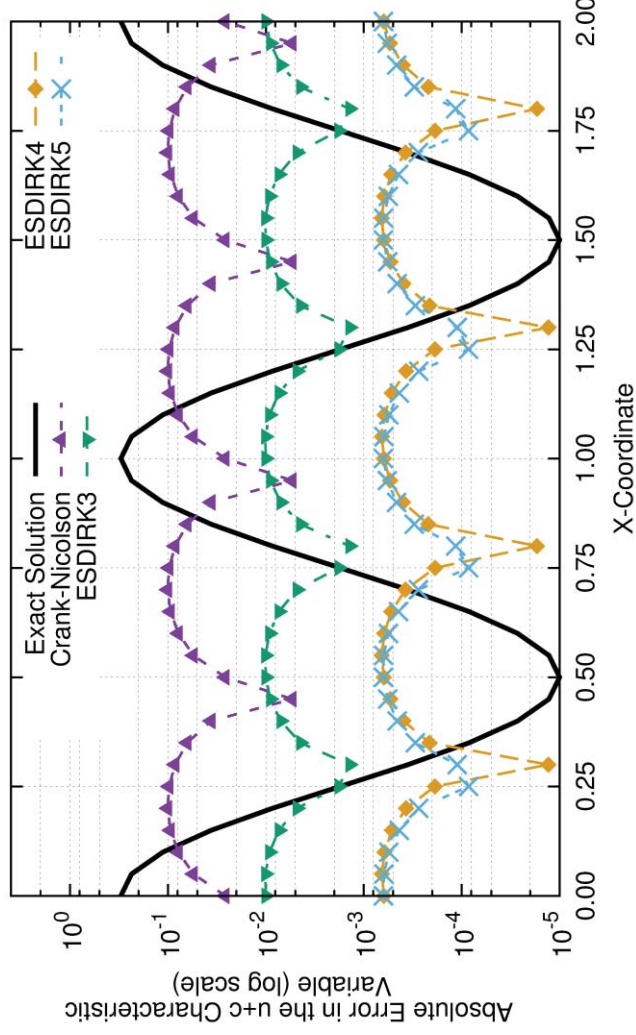
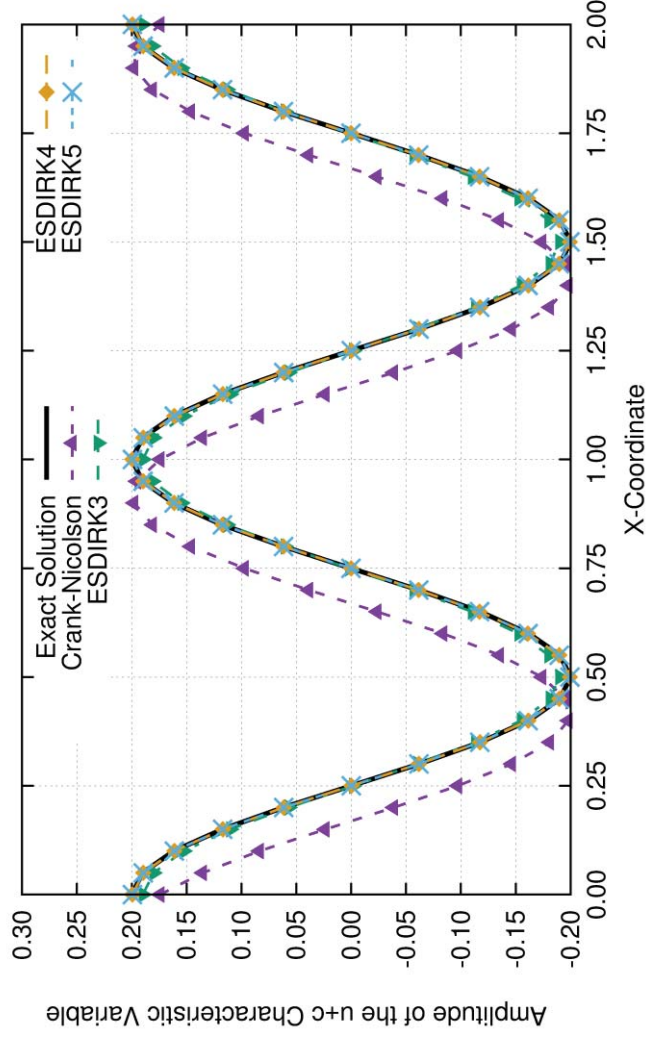
$$\text{where } \hat{\delta} = 0.01$$

- **More results in the paper**



1-D, $CFL = 1.0$, 10 Periods

Scheme	Dissipation Error		Dispersion Error	
	VNA	Simulation	VNA	Simulation
Crank-Nicolson	3.05×10^{-3}	1.00×10^{-2}	8.11×10^{-2}	8.11×10^{-2}
ESDIRK3	5.02×10^{-2}	5.02×10^{-2}	1.51×10^{-3}	1.53×10^{-3}
ESDIRK4	3.13×10^{-3}	3.13×10^{-3}	1.50×10^{-4}	1.58×10^{-4}
ESDIRK5	3.14×10^{-3}	3.14×10^{-3}	6.78×10^{-5}	6.90×10^{-5}

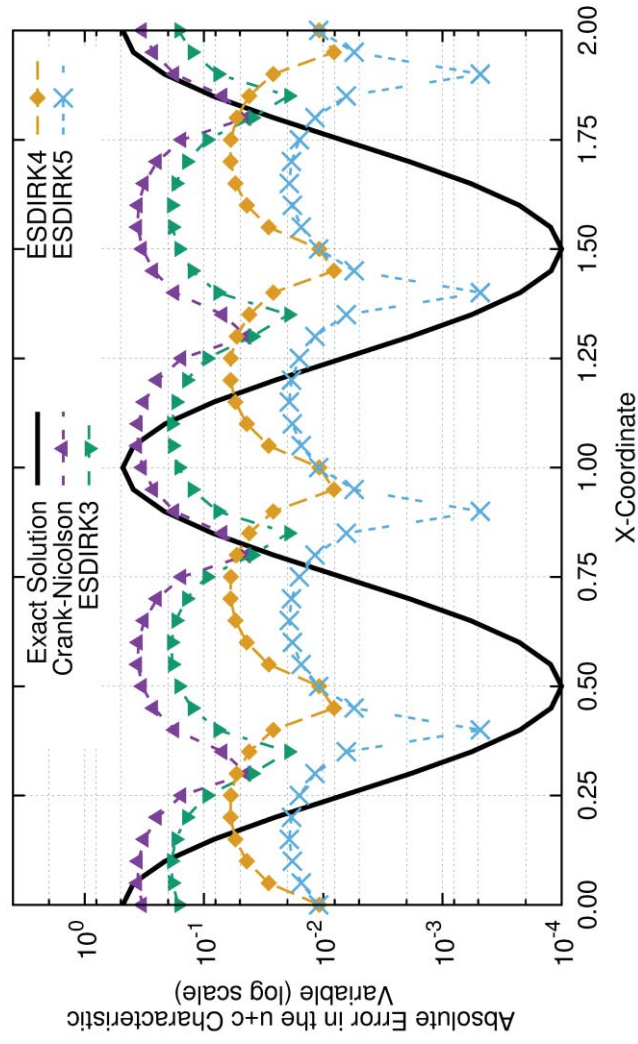
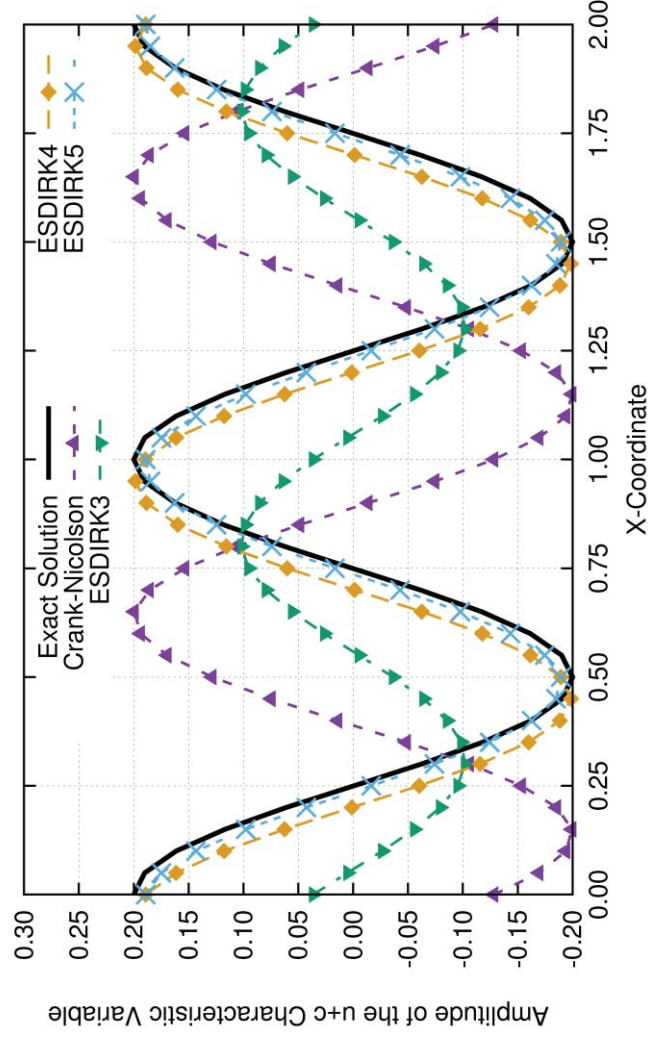




1-D, $CFL = 10.0$, 1 Period



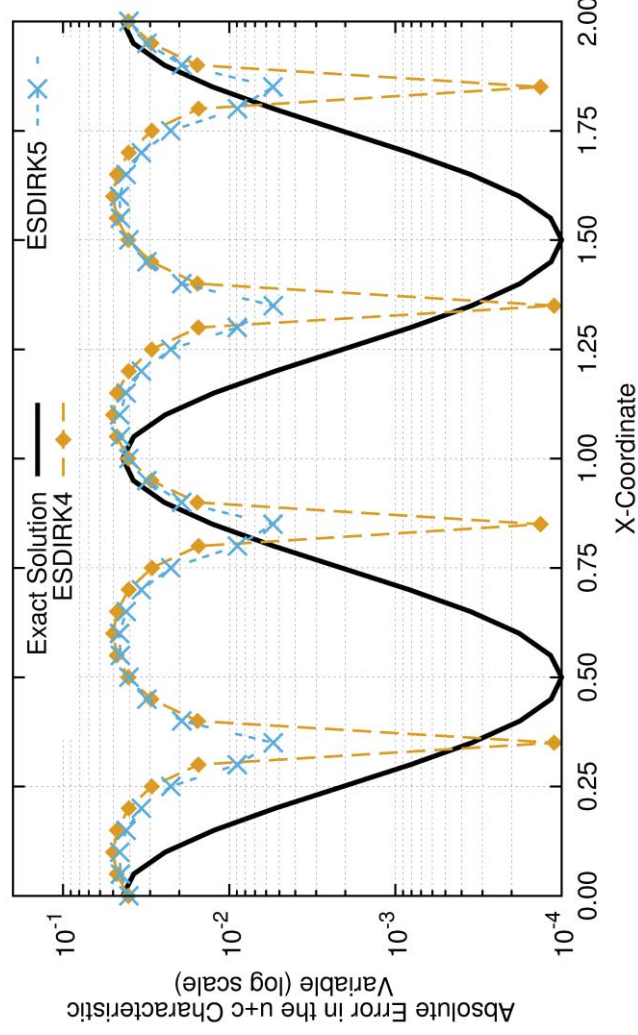
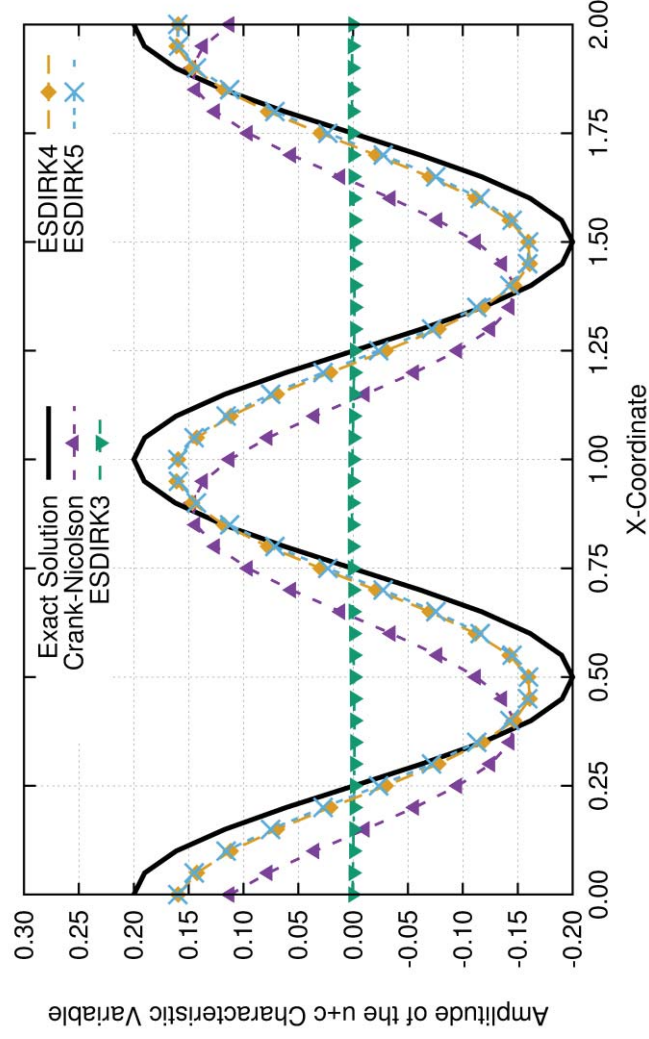
Scheme	Dissipation Error		Dispersion Error	
	VNA	Simulation	VNA	Simulation
Crank-Nicolson	9.02×10^{-5}	2.44×10^{-3}	3.61×10^{-1}	3.61×10^{-1}
ESDIRK3	4.99×10^{-1}	4.90×10^{-1}	1.92×10^{-1}	1.92×10^{-1}
ESDIRK4	7.22×10^{-3}	7.25×10^{-3}	4.90×10^{-2}	4.90×10^{-2}
ESDIRK5	5.10×10^{-2}	5.46×10^{-2}	1.38×10^{-2}	1.39×10^{-2}





1-D, $CFL = 1.0$, 1000 Periods

Scheme	Dissipation Error		Dispersion Error	
	VNA	Simulation	VNA	Simulation
Crank-Nicolson	2.63×10^{-1}	2.65×10^{-1}	8.11×10^0	8.10×10^0
ESDIRK3	9.94×10^{-1}	9.94×10^{-1}	1.51×10^{-1}	1.00×10^{-1}
ESDIRK4	2.69×10^{-1}	1.95×10^{-1}	1.50×10^{-2}	3.00×10^{-2}
ESDIRK5	2.70×10^{-1}	2.01×10^{-1}	6.78×10^{-3}	2.50×10^{-2}





3-D Isentropic Vortex

- **Free-stream Mach number of 0.5**

$$\rho_{\infty} = 1.0 \frac{\text{kg}}{\text{m}^3}, \quad \rho u_{\infty} = 200.0 \frac{\text{kg}}{\text{m}^2 \cdot \text{s}}, \quad \rho v_{\infty} = 0.0 \frac{\text{kg}}{\text{m}^2 \cdot \text{s}}, \quad \rho w_{\infty} = 0.0 \frac{\text{kg}}{\text{m}^2 \cdot \text{s}}, \quad \rho e_{0,\infty} = 305714.3 \frac{\text{kg}}{\text{m} \cdot \text{s}^2}$$

$$R_{\infty} = 287.11 \frac{\text{J}}{\text{kg} \cdot \text{K}} \text{ and } \gamma = 1.4$$

- **Perturbation - 11 points across the vortex**

$$\delta u = -\sqrt{R_{\infty} T_{\infty}} \frac{\alpha}{2\pi} (y - y_0) e^{\phi(1-r^2)}$$

$$\delta v = \sqrt{R_{\infty} T_{\infty}} \frac{\alpha}{2\pi} (x - x_0) e^{\phi(1-r^2)}$$

$$\delta T = T_{\infty} \frac{\alpha^2 (\gamma - 1)}{16\phi\gamma\pi^2} e^{2\phi(1-r^2)}$$

$$\alpha = 4 \text{ and } \phi = 1$$

Vortex center: (x_0, y_0)

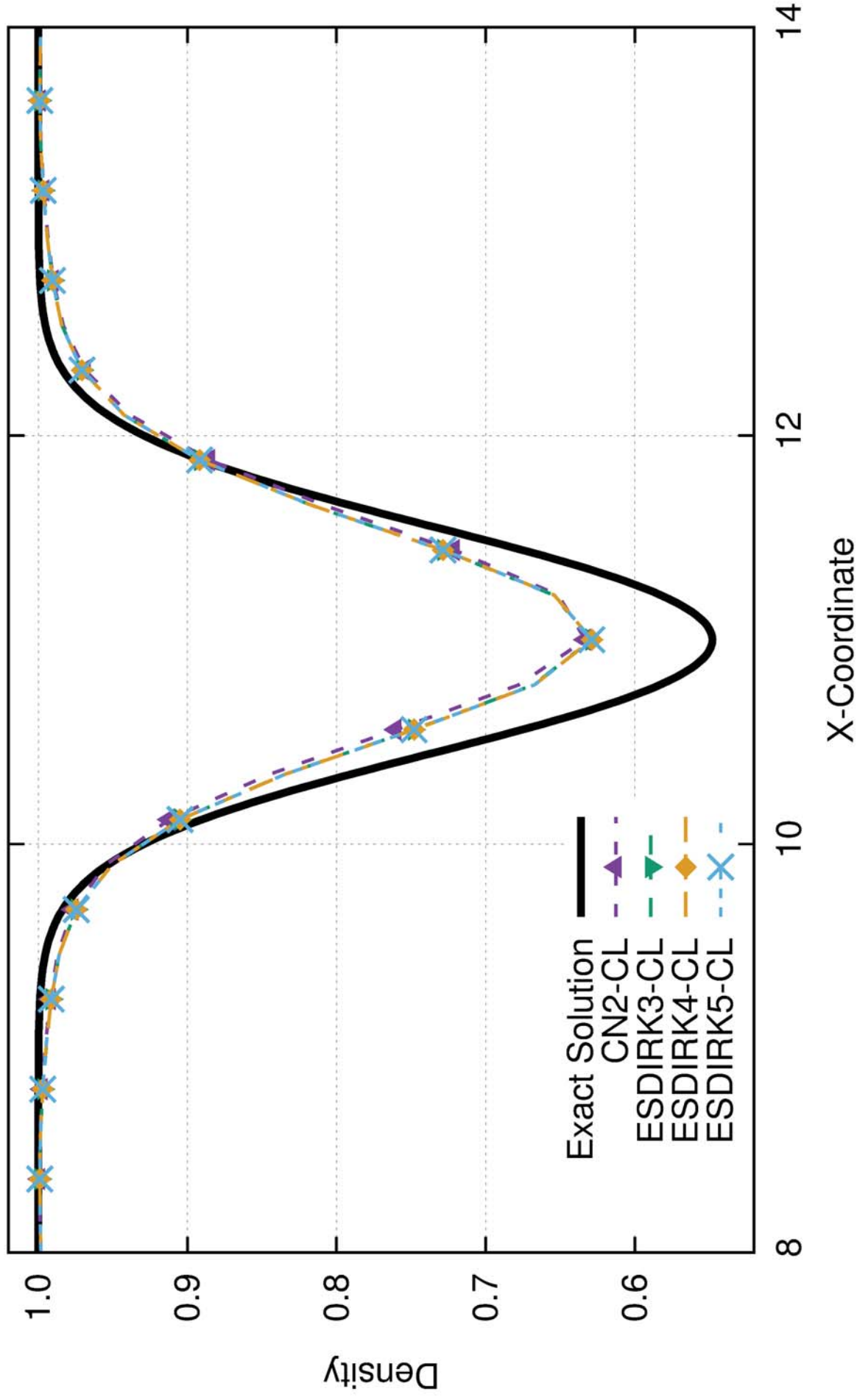
$$r = \sqrt{(x - x_0)^2 + (y - y_0)^2}$$



- **More results in the paper**

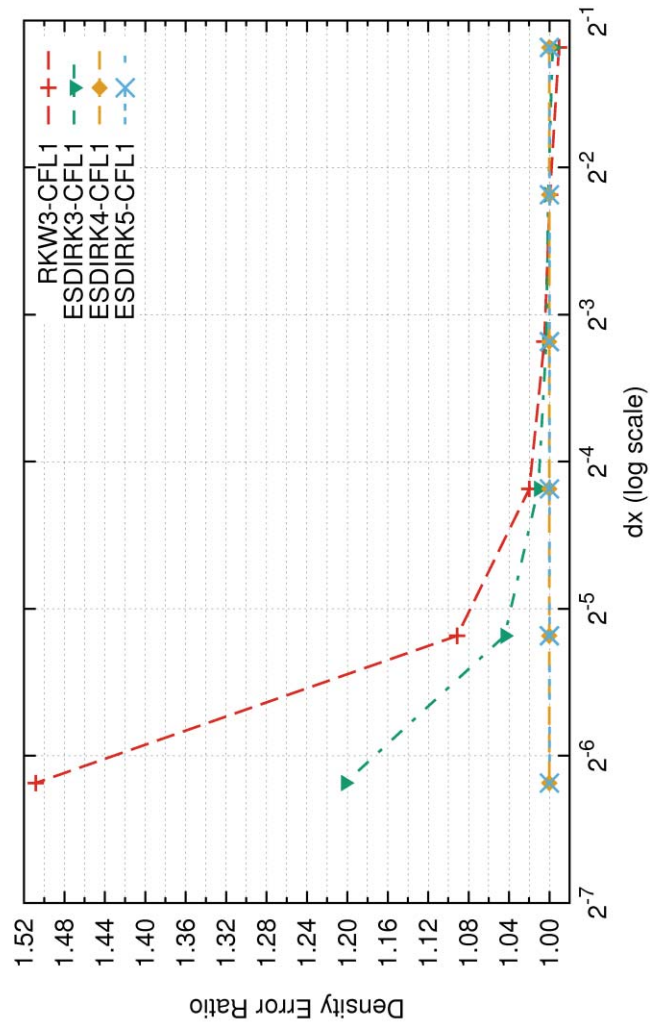
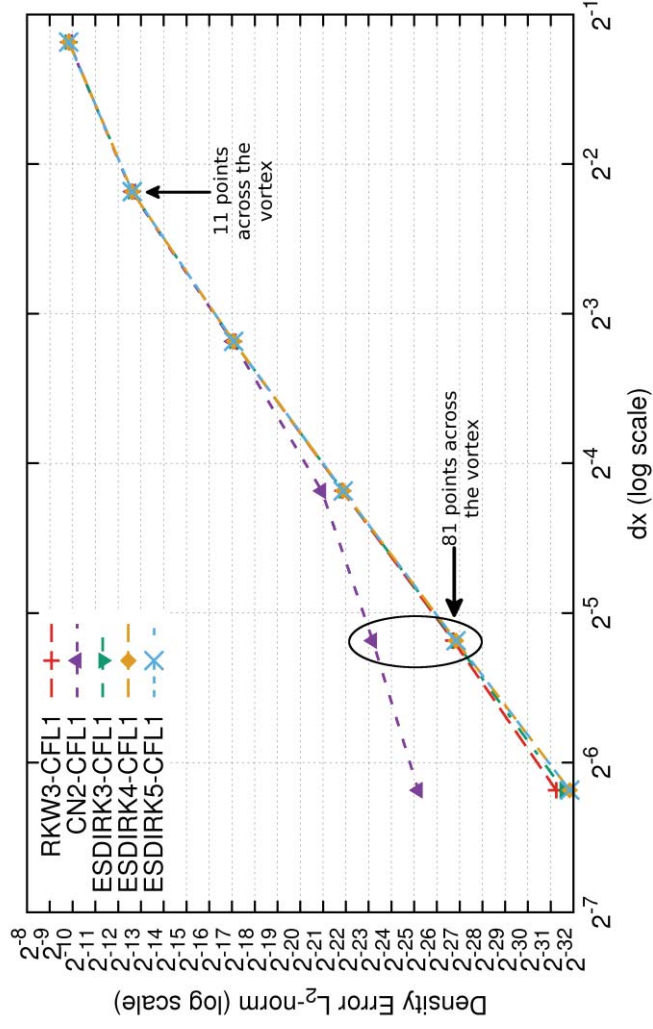


3-D, $CFL = 1.0$, 40 Lengths, 11 Points Across the Vortex



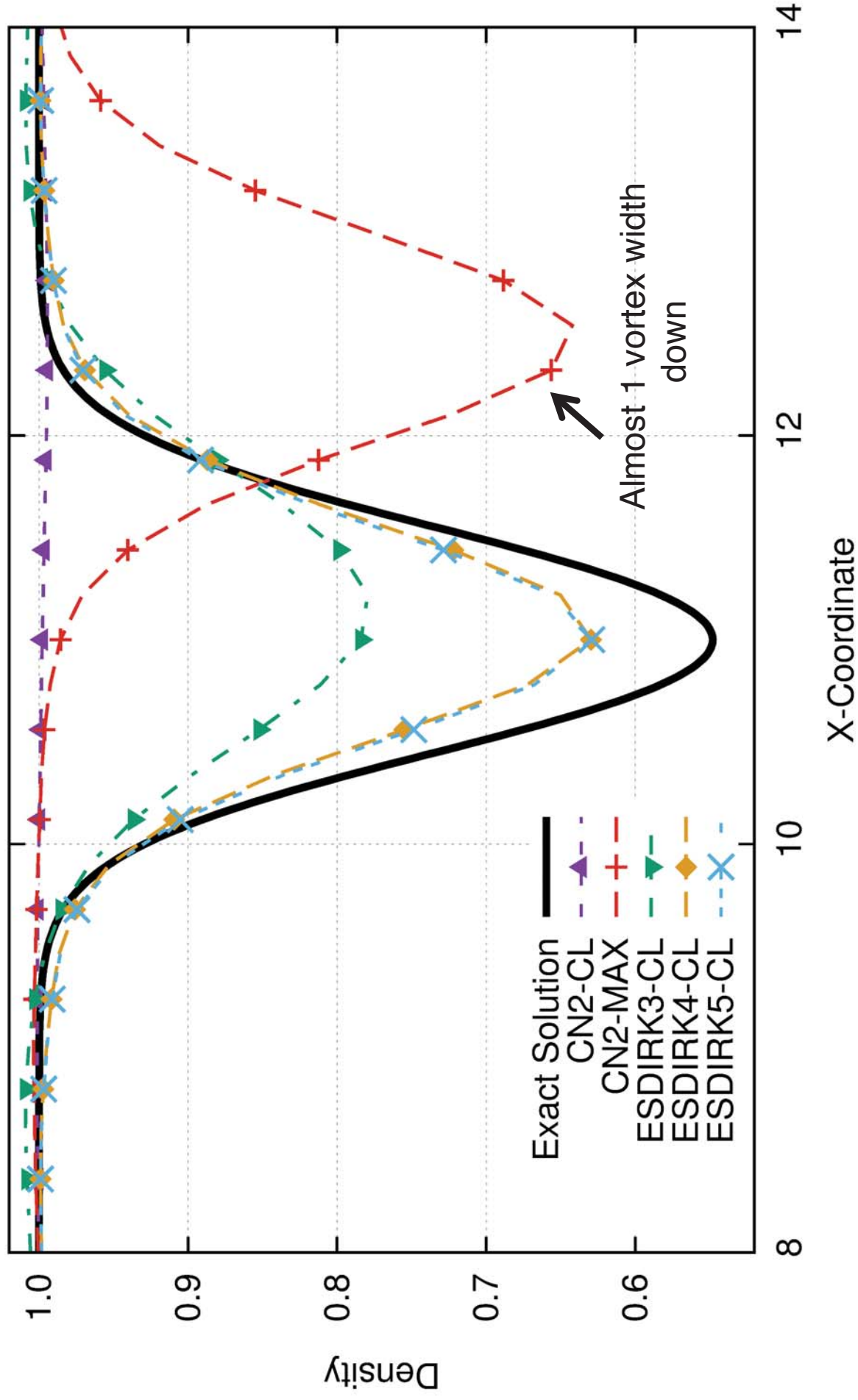


3-D, $CFL = 1.0$ Different Resolutions





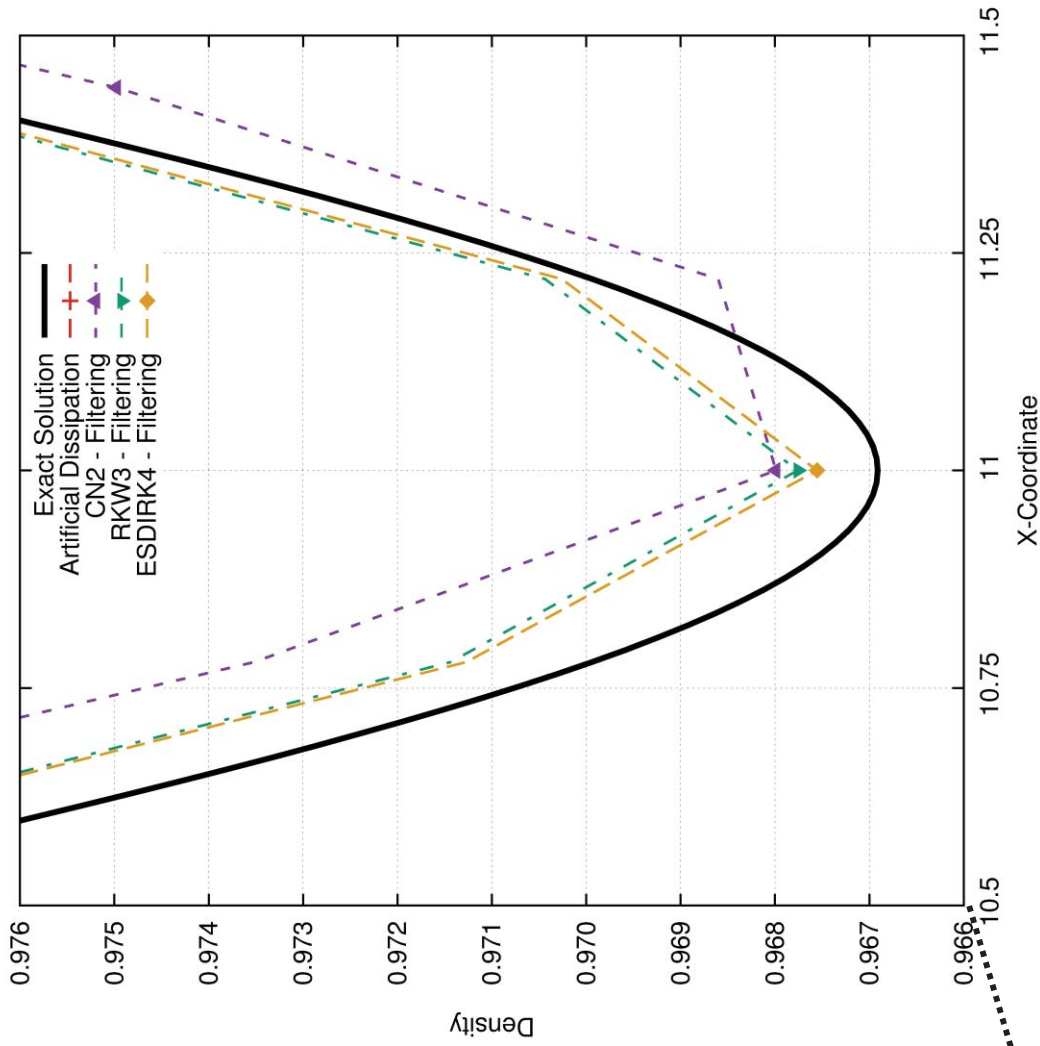
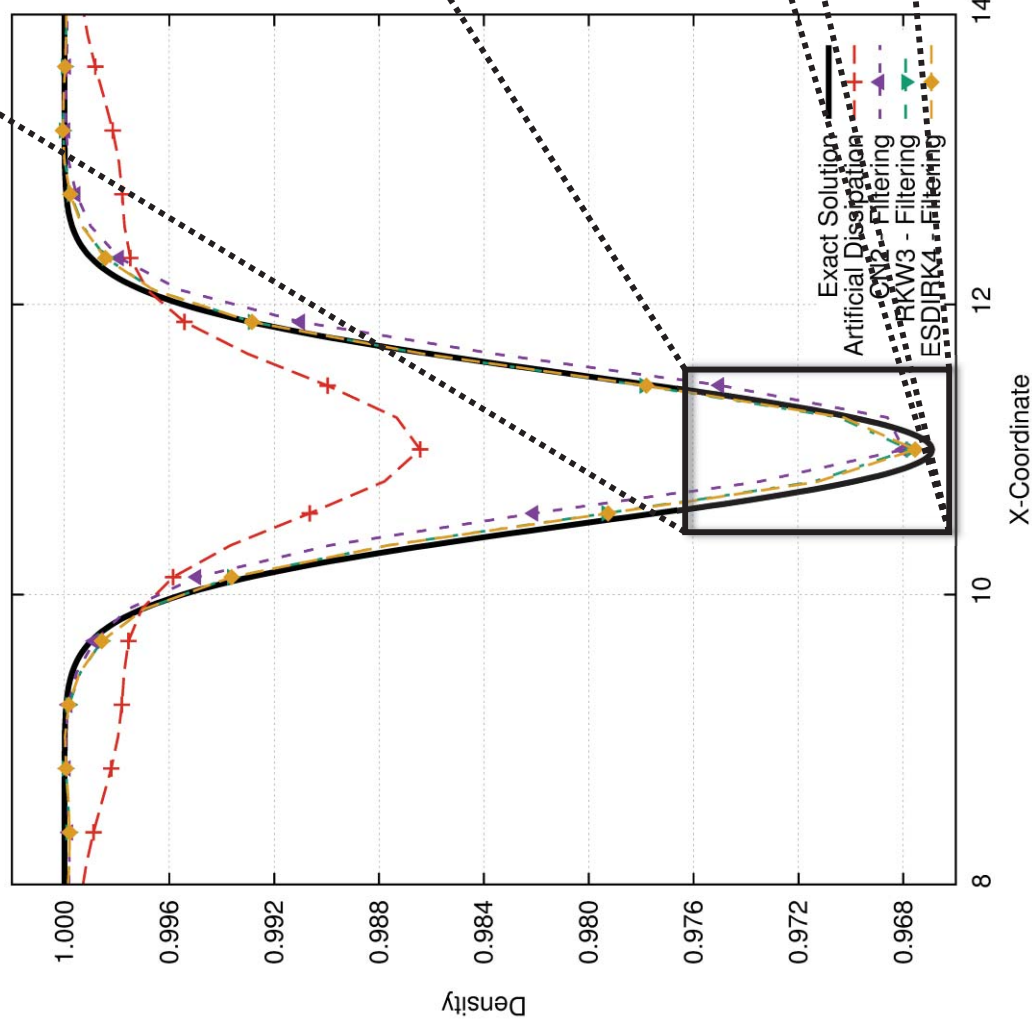
3-D, $CFL = 8.0$, 40 Lengths, 11 Points Across the Vortex





Sneak Peak: Filtering

11 points across the vortex
 $CF_L = 1.0$
80 vortex widths convection





Conclusions

- ***2nd- and 3rd-order time integrators for 5th-order spatial schemes are inadequate***

- The same order of spatial and temporal discretizations is preferable
- However, ESDIRK5 is not much better than ESDIRK4
 - 7 implicit stages vs. 5 implicit stages

- **Higher-order time integrators:**

- Do not show significant improvement on coarse grids at CFL of one
- Are better at high CFL number
- Are better on highly refined grids

- **Spatial error usually dominates for typical CFL numbers and grid resolutions**

- Central difference plus artificial dissipation schemes are inadequate





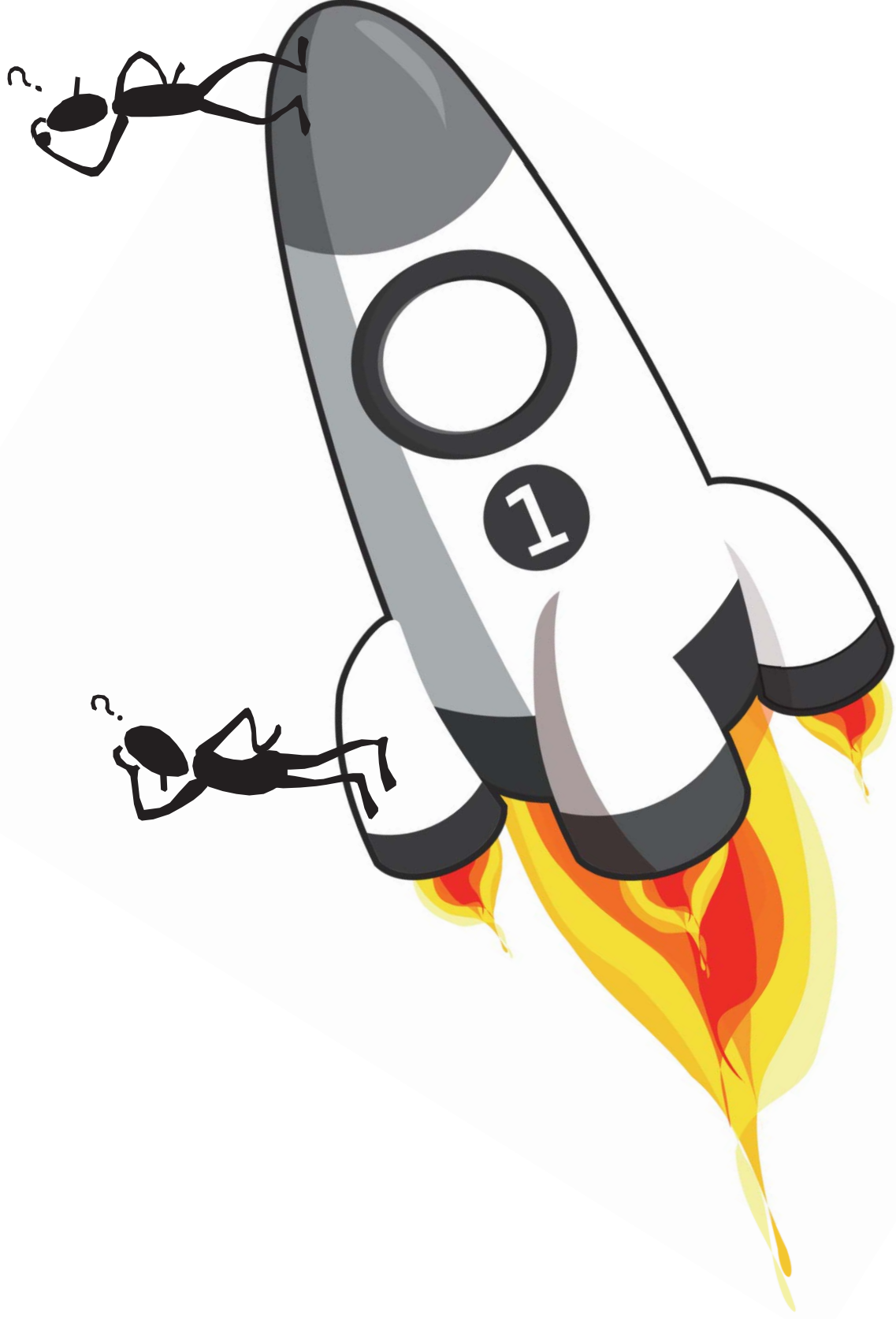
Future Work



- **Implement more accurate spatial schemes of the same orders of accuracy**
 - Compact-difference schemes
 - Filtering schemes
- **Derive better ESDIRK schemes tailored to the desired dissipation and dispersion properties**
- **Add preconditioning to take maximum advantage of the ESDIRK time integrators for stiff problems**
 - Improved convergence efficiency
 - Improved solution accuracy



Questions???





Extra Slides





3-D, $CFL = 8.0$ Different Resolutions

